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New functionalities of Versions 5.0 and 5.1 of the TFEL/MFront project and Versions 3.0 and 3.1 of the MGIS project

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Abstract — As part of the open-source TFEL project, MFront simplifies the implementation of complex mechanical behaviours efficiently and portably across various finite element and FFT solvers. This paper highlights important new features introduced in TFEL/MFront Versions 5.0 and 5.1. It also outlines how the MFrontGenericInterfaceSupport project enables straightforward integration of MFront behaviours into a range of open-source or commercial solvers

Keywords: Constitutive equations, Material knowledge management, Homogenization

Introduction

The projects TFEL/MFront and MGIS have been actively developed since the talk given at the last session of this conference (1), where Version 4.2 of TFEL/MFront and Version 2.0 of MGIS were presented. Those new developments have been made with the contributions and feedback of a large community of academic and industrial users, as demonstrated by the various talks at the MFront user days¹ and the list of publications using MFront².

This paper is devoted to highlighting a selected set of features introduced in versions 5.0 and 5.1 of the TFEL/MFront project and versions 3.0 and 3.1 of the MGIS project³.

This paper is organized as follows:

- Section 1 provides an overview of TFEL, MFront, MTest, and MGIS.
- Section 2 provides a description of the main new features in TFEL of Versions 5.0 and 5.1. and in MGIS of Versions 3.0 and 3.1.
- Section 3 provides a description of some side projects such as MFrontGallery and TFELMathEnzyme.

1 Overview of TFEL, MFront, MTest and MGIS

The TFEL project provides mathematical libraries that are the basis of the MFront code generator and the MTest solver (2). It is an open-source collaborative development of the French Alternative

¹<https://github.com/thelfer/tfel-doc/tree/master/MFrontUserDays>

²<https://thelfer.github.io/tfel/web/publications.html>

³The interested reader may refer to the release notes of those versions available on the website of each project for a comprehensive and detailed description.

Energies and Atomic Energy Commission (CEA) and Électricité de France (EDF) within the framework of the PLEIADES platform (3).

TFEL/MFront is available on a large number of platforms, including Linux, macOS, Windows, FreeBSD with various C++ compilers (gcc, clang, Microsoft's Visual Studio, NVIDIA's nvhpc, and Intel's icpx). TFEL/MFront can be installed in several popular package managers, including spack, conda, and homebrew. Moreover, it is distributed with the Cast3M and code_aster solvers.

1.1 The TFEL/Math library

The TFEL/Math library provides a linear algebra engine with mathematical objects (tensors of arbitrary orders) and operations on those objects required to express the constitutive equations in an efficient and natural manner i.e., as close as possible to the mathematical expressions common in the engineering sciences. These mathematical objects can have units, allowing the compiler to perform dimensional analysis at compile-time. A framework to build nonlinear solvers for small-sized problems. Efficient and robust implementations of several classical non linear algorithms (Newton-Raphson, Broyden, Levenberg-Marquart, etc.) are provided.

This library has been ported to GPUs and tested in the main programming models (CUDA, HIP, SYCL, Kokkos, etc.). Section 3.3 describes how the Enzyme library can be used to add automatic differentiation to TFEL/Math.

1.2 The TFEL/Material library

The TFEL/Material library provides implementations of various utility functions frequently required in constitutive modelling (computation of the Lamé coefficients, computation of the Hill tensors). In particular, computations of many popular stress criteria and their derivatives with respect to the stress tensor (Hill 1948, Hosfort 1978, Gurson 1977, Gurson-Tvergaard-Needlman 1984, Barlat 2004, Mohr-Coulomb, etc.) have been implemented.

This library has been recently extended to provide useful functions for mean-field homogenization, as described in Section 2.1.

1.3 The MFront code generator

MFront translates a set of closely related domain-specific languages into plain C++ on top of the TFEL libraries.

Those languages are meant to be easy to use and learn by researchers and engineers. They cover three kinds of material knowledge: material properties (Young's modulus, thermal conductivity, etc.), mechanical behaviours and simple point-wise models (such as material swelling under irradiation used in fuel performance codes). Concerning behaviours, the following kinds of behaviours are supported:

- small and finite strain mechanical behaviours.
- cohesive zone models.
- generalised behaviours, such as the one encountered in higher order theories, Cosserat media, heat transfer, strongly coupled thermomechanical analysis, damage gradient models, etc.

Authors of MFront pay particular attention to the robustness, reliability and numerical efficiency of the generated code, in particular for mechanical behaviours. Various benchmarks show that MFront implementations are competitive with native implementations available in the Cast3M, code_aster, Europlexus, Abaqus/Standard, Abaqus/Explicit (4) solvers and in the fuel performance codes Cyrano3 (5) and Galileo (6).

Portability is also a very important issue: a behaviour written in MFront shall be usable in any solver for which an interface exists. In addition to the aforementioned solvers, interfaces exist

for: [Ansys](#), [ZMat](#), [CalculiX](#), [DianaFEA](#).

1.4 The generic interface and the MFrontGenericInterfaceSupport project

To limit the number of interfaces supported by MFront, an interface called `generic` has been introduced, along with the [MFrontGenericInterfaceSupport project](#) (MGIS), which provides solver developers tools (functions, classes, bindings, etc...) to handle behaviours generated by this `generic` interface.

The MFrontGenericInterfaceSupport project has already been integrated or tested in many solvers (7), including [code_aster](#), Manta (8), [MFEM-MGIS](#) (9), [OpenGeoSys](#) (10), [dolfinx_materials](#), etc.

2 New features

Behind the scenes, Version 5.0 of TFEL and Version 3.0 of MGIS were rewritten to take advantage of C++-20. This section highlights some noticeable new features from the end user's point of view provided by these two projects.

2.1 The TFEL/Material/Homogenization library

[Homogenization tools](#) have been added to the TFEL library and can be used in MFront. These tools include Hill tensors and localisation tensors, classical homogenization bounds and computation of homogenized stiffness by classical schemes, for very general microstructures.

2.1.1 Eshelby tensors, Hill tensors and localisation tensors

The computation of Eshelby tensors or Hill tensors or localisation tensors is analytically possible (11) when the inclusion is ellipsoidal and embedded in an isotropic matrix.

Three cases are considered in the library: spherical, ellipsoidal and spheroidal (or axisymmetrical) inclusions. Some examples are given below.

```
using namespace tfel::material::homogenization::elasticity;
const auto S0 = computeSphereEshelbyTensor<stress>(nu0);

//IMO is a YoungNuModuli object, giving the isotropic
//moduli of the matrix phase
//n_a gives the orientation of the spheroid
const auto IMO=YoungNuModuli<stress>(EO,nu0);
const auto PO = computeAxisymmetricalHillPolarisationTensor<stress>(IMO,n_a,e);

//here, if the axes a,b,c are all different, two vectors n_a and n_b
//are necessary to precise the orientation of the ellipsoid
const auto IMi=YoungNuModuli<stress>(Ei,nui);
const auto A = computeLocalisationTensor<stress>(IMO,IMi,n_a,a,n_b,b,c);
```

These tensors can also be computed when considering plane strain elasticity, or anisotropic elasticity of inclusions.

2.1.2 Computation in anisotropic matrix

When the inclusions are embedded in a fully anisotropic matrix, the analytical computation is no more possible and a numerical integration on a bi-dimensional domain is carried out to compute these tensors.

They can be computed as follows:

```

// With an anisotropic matrix, the elasticity C0 is a 'st2tost2' object
const auto S0 = computeAnisotropicEshelbyTensor<stress>(C0,n_a,a,n_b,b,c);
const auto P0 = computeAnisotropicHillTensor<stress>(C0,n_a,a,n_b,b,c);

//here Ci_loc is a 'st2tost2' object giving the inclusion elasticity
const auto A =
    computeAnisotropicLocalisationTensor<stress>(C0_glob,Ci_loc,n_a,a,n_b,b,c);

```

The user can also control the precision of the integration by providing some additional arguments. Moreover, the tensors can be computed when considering plane strain elasticity.

2.1.3 Homogenization bounds

Different homogenization bounds are available for an arbitrary number of phases, in dimension 2 or 3: Reuss bounds, Voigt bounds and Hashin-Shtrikman bounds (for isotropic phases).

2.1.4 Homogenization schemes

The homogenized stiffness tensors given by classical mean-field homogenization schemes are available for different types of microstructure.

A first set of functions is defined when considering simple particulate microstructures, biphasic, with isotropic phases. They do not require the instantiation of microstructure objects and are more suited to fast computation.

Different distributions of ellipsoids can be considered:

- spheres (no orientations)
- oriented ellipsoids (two vectors $\underline{n}_a, \underline{n}_b$ define the orientation)
- uniform isotropic distribution of orientations (the ellipsoids have no preferential orientation)
- transverse isotropic distribution of orientations (one axis \underline{n}_a of the ellipsoid is fixed, the others are uniformly distributed in the transverse plane)

For example, we can do:

```

const auto IM0=YoungNuModuli<stress>(EO,nu0);
const auto IMi=YoungNuModuli<stress>(Ei,nui);
const auto KG_DS = computeSphereDiluteScheme<stress>(IM0,f,IMi);

//Here the ellipsoid is not necessarily a spheroid, and 'TransverseIsotropic'
//means that the axis relative to length a has a fixed orientation (given by
//n_a) and the two other axes rotate
const auto C_DS =
    computeTransverseIsotropicDiluteScheme<stress>(IM0,f,IMi,n_a,a,b,c);

const auto C_MT =
    computeOrientedMoriTanakaScheme<stress>(IM0,f,IMi,n_a,a,n_b,b,c);

//Here the distribution is isotropic in the sense that the ellipsoids have
//random orientations with a uniform probability
const auto KG_MT = computeIsotropicMoriTanakaScheme<stress>(IM0,f,IMi,a,b,c);

```

Ponte-Castaneda and Willis scheme (12) is also available:

```

//Here, a `Distribution` object (which defines the distribution of inclusions)
//must be created
Distribution<stress> D = {.n_a = n_a, .a = a, .n_b = n_b, .b = b, .c = c};
const auto C_PCW = computeIsotropicPCWScheme<stress>(IM0,f,IMi,a,b,c,D);

```

Some other details are provided in the [documentation](#).

2.1.5 Homogenization of complex microstructures

In some cases (multi-phasic microstructures) the functions described above are not sufficient to compute homogenized stiffness tensors. Hence, more complex features can be introduced by creation of `ParticulateMicrostructure` objects. It permits to consider an arbitrary number of phases, each phase being a distribution of ellipsoidal inclusions with very general properties.

For example, a construction of such a microstructure can be:

```
const auto IMO=tfel::material::KGModuli<stress>(1e7,1e7);
const auto microstructure=ParticulateMicrostructure(IMO);

Sphere<length> sphere();
Spheroid<length> spheroid(a,b);

const auto KGi=tfel::material::KGModuli<stress>(Ki,Gi);
SphereDistribution<stress> sphere_distribution(sphere,f,KGi);
IsotropicDistribution<stress> spheroid_distribution(spheroid,f,KGi);

microstructure.addInclusionPhase(sphere_distribution);
microstructure.addInclusionPhase(spheroid_distribution);
```

Three classical schemes are implemented for these microstructures, dilute, Mori-Tanaka and self-consistent.

Hence, we can do

```
auto hm_MT=computeMoriTanaka<3u,stress>(microstructure);
//Some features like 'homogenized_stiffness' or
//'mean_strain_localisation_tensors' can be obtained:
auto Chom=hm_MT.homogenized_stiffness;
auto A_i=hm_MT.mean_strain_localisation_tensors;
```

These latter attributes have been implemented in view of non-linear schemes based on linear comparison composites.

2.1.6 Python module `tfel.material.homogenization`

The new functionalities described above are also available via the Python package `tfel.material.homogenization`.

2.2 Main improvements to MFront

2.2.1 Warnings

Many warnings have been added to detect potential misuses of MFront or known bad practices. A typical example of this feature is the following:

```
$ mfront --interface=generic Plasticity.mfront
[warning]: using the default value for the convergence threshold.
This value is generally considered too loose.
You may want to consider a more stringent value (1e-14 is a good choice).
See the `@Epsilon` keyword for details.
```

The user has many ways of controlling how warnings are treated, or how to activate/deactivate them.

2.2.2 Strain rate sensitive isotropic hardening rule in the StandardElastoViscoplasticity brick

The StrainRateSensitive isotropic hardening rule is defined by:

$$R(p, \dot{p}) = R_0(p) R_{rs}(\dot{p}),$$

where:

- $R_0(p)$ is the yield radius corresponding to an infinitely slow loading. It can be built by summing any isotropic hardening rule already implemented in the StandardElastoViscoPlasticity brick.
- $R_{rs}(\dot{p})$ is a correction describing the strain rate sensitivity. $R_{rs}(0)$ must be equal to 1.

This isotropic hardening rule can be parametrised using the following options:

- `rate_independent_isotropic_hardening`: this option introduces a contribution to $R_0(p)$. This option can be repeated multiple times.
- `rate_sensitivity_factor`: this option introduces the rate sensitivity factor $R_{rs}(\dot{p})$.

In Version 5.1, two classical rate sensitivity factors have been implemented, namely CowperSymonds (13) and JohnsonCook (14). The following snippet illustrates this feature:

```
@Brick StandardElastoViscoPlasticity{
  stress_potential : "Hooke" {young_modulus : 210e9, poisson_ratio : 0.3},
  inelastic_flow : "Plastic" {
    criterion : "Mises",
    isotropic_hardening : "StrainRateSensitive" {
      rate_independent_isotropic_hardening : "Voce" {
        RO : "Q1 * (1 - Q2)", Rinf : "Q1", b : "Q3"
      },
      rate_sensitivity_factor :
        "CowperSymonds" {dp0 : "dp0cs", n : "ncs", Rs_eps : 1e-8}
    }
  }
};
```

2.2.3 Behaviour variables

A behaviour variable is a practical way to call another MFront behaviour from a main behaviour. A behaviour variable can be declared as follows:

```
@BehaviourVariable first_phase_plastic_behaviour {
  file: "Plasticity.mfront",
  variables_suffix: "1",
  external_names_prefix: "FirstPhase",
  store_gradients: true,
  store_thermodynamic_forces: true,
  shared_material_properties: {".+"},
  shared_external_state_variables: {".+"}
};
```

The main point is to declare what variables are shared with the main behaviour and the behaviour variable. In the previous example, the material properties are all shared.

Behaviour variables are useful in many contexts:

- It allows switching from a numerical implementation to another, for instance from a fast implementation to a robust one if the fast one diverges.

- It allows easy implementation of various non-linear homogenization schemes. Tutorials are available on the TFEL website for:
 - Implementing [the Sachs/Reuss homogenization scheme](#).
 - Implementing [the Taylor/Voigt homogenization scheme](#).
 - Implementing [the \$\beta\$ -rule homogenization scheme](#).

2.2.4 Extension of the @Model keyword

In previous versions, the @Model keyword allowed calling from a behaviour point-wise models using the historical Model DSL.

The @Model keyword now allows using point-wise models implemented using the following DSLs: DefaultModel, RungeKuttaModel and ImplicitModel. In this case, a behaviour variable is automatically associated with every point-wise model. This behaviour variable shares all its material properties and external state variables with the calling behaviour. Every persistent variable of the point-wise model is declared as an auxiliary state variable in the calling behaviour, and a local variable is declared, which contains the increment of this variable over the time step.

This feature allows easy coupling of behaviours with phase transition, swelling under irradiation, etc.

2.3 The MGIS/Function library

The main new feature of MGIS is the MGIS/Function[^functions] library, which has been introduced to provide standard mechanical post-processings based on the TFEL/Math and TFEL/Material libraries. MGIS/Function allows reusing the large amount of documented and verified functionalities provided by those libraries at the structural scale, including: rotation from/to material frame, conversion between stress measures, Hencky and Green-Lagrange strains, Tresca, von Mises, Hosford, Hill, Barlat equivalent stresses, principal values, Lode’s angle, etc.

[^functions] A function denote a set of values associated with the elements (nodes, quadrature points, cells) of a discretized space. Functions are often called **fields** in many solvers.

The following snippet computes the Cauchy stress in the global frame from the first Piola-Kirchhoff stress known in the material frame.

```
const auto evaluator = pk1_function | as_tensor<3> |
    from_pk1_to_cauchy (F_function | as_tensor<3>) |
    rotate_backwards (R_function | as_matrix<3,3>);
const auto ok = assign(ctx, sig | as_stensor<3>, evaluator);
```

The library is developed in C++-20 with high-quality requirements and strives to be **constexpr** friendly, memory-safe, thread-safe, exception-safe, and **GPU-friendly**.

The data structures of the functions depend on the targeted solver, as well as the implementation of the **assign**, which depends on the programming model chosen by the targeted solver (OpenMP, CUDA, SYCL, Kokkos, etc.).

For standard data structures, such as the one used by Numpy’s array, so-called **views** are provided allowing direct usage of the library. In this case, an implementation of the **assign** algorithm is provided by the parallel version of the Standard library. Depending on the compiler and implementation of the standard library, various parallel programming models are used (multithreading and GPU-offloading).

3 A description of some side projects of TFEL/MFront

Aside from MGIS, several side projects built on top of TFEL/MFront have been actively developed.

3.1 MFrontGallery

The [MFrontGallery project](#) addresses the management of MFront implementations, including their compilation, unit testing, and deployment (15).

The project has two main, almost orthogonal, objectives:

1. Show how solver developers may provide their users a set of ready-to-use (mechanical) behaviours that can be parametrized to meet specific needs.
2. Describe how to set up a high-quality material knowledge management project based on [MFront](#), capable of meeting the requirements of safety-critical studies.

While the first objective is common to all (mechanical) solvers, the originality of the MFrontGallery project is to address the second goal. In summary, the project provides:

- A [CMake](#) infrastructure that can be replicated in (academic or industrial) [derived projects](#), which allows:
 - compiling MFront sources using all supported interfaces.
 - executing unit tests based on [MTest](#) which generate XML result files conforming to the [JUnit](#) standard, compatible with continuous integration platforms such as [jenkins](#).
 - generating documentation associated with the stored implementations.
- A [documentation of best practices](#) for handling material knowledge implemented with MFront, such as use of consistent unit systems, bound-aware physical quantities, consistent tangent operators, and others.
- A set of high-quality MFront implementations.

3.2 Damage indicators for uncoupled analysis of brittle and ductile failures

The [FailureCriteria project](#) provides MFront’s implementations of various criteria to predict brittle and ductile failure. These implementations can be used in uncoupled analyses as a post-processing, or in coupled analyses where the criteria are, for example, used along with an element-deletion strategy. The following criteria are available:

- for brittle analyses: Beremin et al. (16), Ruggieri and Dodds (17), and Forget, Marini and Vincent (18).
- for ductile failure: Freudenthal (19), Cockcroft and Latham (20), Rice and Tracey (21), Hancock and McKenzie (22), Johnson and Cook (23), Huang (24), and Bai and Wierzbicki (25).

This library can be used directly in solvers interfaced with MGIS. Using MGIS in Python allows using the library when simulations’ data are available as NumPy’s arrays. As an example, the documentation of the library includes a tutorial showing how to post-process simulation results exported from Cast3M as VTK files.

3.3 The TFELEMathEnzyme library

The TFELEMathEnzyme library leverages the [Enzyme automatic differentiation tool](#) (26, 27) to extend the TFELE/Math library ⁴.

To illustrate the use of this library, let us consider the Hosford equivalent stress defined as:

$$\sqrt[2]{(\sigma_I - \sigma_{II})^2 + (\sigma_I - \sigma_{III})^2 + (\sigma_{II} - \sigma_{III})^2}$$

where σ_I , σ_{II} and σ_{III} are the eigenvalues of the stress tensor. Implementing a plastic behaviour using this equivalent stress requires computing its first and second derivatives, the

⁴Enzyme is a plugin of the LLVM infrastructure on top of which is built the clang compiler. Enzyme generates derivatives of functions by automatic differentiation after the optimisations performed by the LLVM infrastructure. This solution is thus specific to this compiler.

implementations of which are complex. Although those computations are already implemented in `TFEL/Material`, it is interesting to see how those computations can be delegated to `Enzyme` through `TFELMathEnzyme`:

```
auto estress = [seps](const StressTensor &s) {
    return computeHosfordStress(s, 100, seps);
};
auto dseq = getDerivativeFunction<Mode::REVERSE, 0>(estress);
auto d2seq = getDerivativeFunction<Mode::REVERSE, 0>(dseq);
```

While early results are encouraging, the `TFELMathEnzyme` library is still very experimental.

Conclusions and future works

Future work aims at enlarging the set of physical features provided by the `TFEL/Math` and `TFEL/Material` libraries and integrating them in `MFront`, in particular through so-called bricks. In particular, a brick dedicated to nonlinear mean-field homogenization is planned.

In parallel, developments regarding GPU's support and automatic differentiation, which are currently experimental in `MFront`, are expected to mature.

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